orientation and others in the twin orientation. A general equation covering this situation is obtained by multiplying equations (A7) and (A8) giving on simplification

$$\varrho^6+(1-3\alpha_{3c})\varrho^3+(1-6\alpha_{hhc}-3\alpha_{3c})=0 \quad \text{for } \alpha\text{'s} \ll 1 \quad \text{(A9)}$$

where terms with squares and higher powers of the fault probabilities as also their cross products have been omitted.

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X-ray Diffraction from Close-Packed Structures with Stacking Faults. III. *hhcc* Crystals

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The kinematical theory of X-ray diffraction by *hhcc* crystals with stacking faults is developed. The intensity distribution in reciprocal space is derived as a function of seven parameters which represent four growth and three deformation fault probabilities. Only reflexions with $H-K\neq 3N$, N an integer, are affected by faulting and exhibit generally changes in integrated intensity, profile peak shift, broadening and asymmetry. It is shown that eleven independent combinations of the seven fault probabilities can be evaluated from the measured profile characteristics.

Introduction

Extensive work has been performed on the derivation of X-ray diffraction effects of faulting in close-packed structures with ranges of influence equal to 2 and 3 (Warren, 1959; Anantharaman, Rama Rao & Lele, 1972). Three structures with a range of influence equal to 4 are possible. Diffraction effects of growth and deformation faults for two of these, namely *hcc* and *hhc* structures, have been treated in earlier papers (Lele, 1974*a*,*b*) while Gevers (1954) has given a general treatment for growth faults in crystals of this type. In the present paper we shall consider the third structure, namely *hhcc*, containing growth and deformation faults.

The 12-layered *hhcc* structure can be considered as a layer structure produced by the regular stacking of close-packed layers in the sequence *ABACBCBACACB*, *A* where the letters *A*, *B* and *C* denote the three possible positions of the close-packed layers and the comma marks the completion of the repeat period. The geometrical structure factors for different *H*, *K*, *L* are given in Table 1. The possible growth and deformation faults along with a different notation due to Nabarro (1967), virtual processes for their formation and stacking sequences containing the faults (indicated by vertical bar) are given in Table 2. The following calculations have been made under assumptions usual in this type of work (see, *e.g.*, Prasad & Lele, 1971).

Diffraction from faulted crystals

Following Warren (1959), the diffracted intensity is given by

$$I(h_3)=\psi^2\sum_m\langle\exp(i\Phi_m)\rangle\exp(2\pi imh_3/12) \quad (1)$$

where

$$\Phi_m=(2\pi/3)(H-K)q_m \quad (2)$$

q_m being a stochastic variate equal to 0, 1 or 2 respectively according as the m layer is A, B or C when the origin layer is A. Cyclic permutation yields the values of q_m for B and C layers at the origin. Further,

$$\langle\exp(i\Phi_m)\rangle=C\varrho^m \quad (3)$$

where ϱ is a solution of the so-called characteristic equation and C can be obtained from the initial conditions. The characteristic equation for growth faults has been obtained by Gevers (1954, equation 12) while that for deformation faults is derived in the Appendix. Combining these two equations, we have finally

$$\varrho^8+\alpha_c\varrho^7+\alpha_{hhc}\varrho^5+(1-\alpha_h-\alpha_c-\alpha_{hhc}-\alpha_{cch}-3\alpha_{4h}-6\alpha_{2hc})\varrho^4-\alpha_c\varrho^3-\alpha_{hhc}\varrho+(1-2\alpha_h-2\alpha_c-2\alpha_{hhc}-2\alpha_{cch}-3\alpha_{4h}-6\alpha_{2hc}-3\alpha_{4c})=0 \quad \text{for } \alpha\text{'s}\ll 1 \quad (4)$$

where α_x is the probability of the occurrence of faults of type x (Table 2). For convenience, the relationship to Gevers' (1954) notation is given below

$$\alpha_h \to (1-\alpha_1);\quad \alpha_c \to \alpha_4;\quad \alpha_{hhc} \to (1-\alpha_3);\quad \alpha_{cch} \to \alpha_2.$$

Solutions of equation (4) may be expressed in the following form

$$\varrho_\nu = Z_\nu \exp(-2\pi i)\left(\frac{\nu}{12}+X_\nu\right) \quad \nu=1,2,4,5,7,8,10,11 \quad (5)$$

where Z_ν and X_ν are real and are given by

$$Z_1=Z_{11}=1-\tfrac{1}{4}(\alpha_h+\alpha_{cch})-\frac{2+\sqrt{3}}{8}(\alpha_c+\alpha_{hhc})-\tfrac{3}{8}(\alpha_{4h}+2\alpha_{2hc}+\alpha_{4c})$$

$$Z_2=Z_{10}=1-\tfrac{1}{4}(\alpha_h+\alpha_{cch})-\tfrac{1}{8}(\alpha_c+\alpha_{hhc})-\tfrac{3}{8}(\alpha_{4h}+2\alpha_{2hc}+\alpha_{4c})$$

$$Z_4=Z_8=1-\tfrac{1}{4}(\alpha_h+\alpha_{cch})-\tfrac{3}{8}(\alpha_c+\alpha_{hhc})-\tfrac{3}{8}(\alpha_{4h}+2\alpha_{2hc}+\alpha_{4c})$$

$$Z_5=Z_7=1-\tfrac{1}{4}(\alpha_h+\alpha_{cch})-\frac{2-\sqrt{3}}{8}(\alpha_c+\alpha_{hhc})-\tfrac{3}{8}(\alpha_{4h}+2\alpha_{2hc}+\alpha_{4c}) \quad (6)$$

$$X_1=-X_{11}=-\frac{1}{16\pi}\{(\alpha_c-\alpha_{hhc})+\sqrt{3}(\alpha_{4h}+2\alpha_{2hc}-\alpha_{4c})\}$$

$$X_2=-X_{10}=\frac{\sqrt{3}}{16\pi}\{(\alpha_c-\alpha_{hhc})+(\alpha_{4h}+2\alpha_{2hc}-\alpha_{4c})\}$$

$$X_4=-X_8=\frac{\sqrt{3}}{16\pi}\{(\alpha_c-\alpha_{hhc})-(\alpha_{4h}+2\alpha_{2hc}-\alpha_{4c})\}$$

$$X_5=-X_7=-\frac{1}{16\pi}\{(\alpha_c-\alpha_{hhc})-\sqrt{3}(\alpha_{4h}+2\alpha_{2hc}-\alpha_{4c})\}.$$

As mentioned earlier the C_ν's can be found from the initial conditions. The latter found by direct evaluation from all possible stacking sequences of eight layers, are given below

$$\langle\exp(i\Phi_0)\rangle=1$$

$$\langle\exp(i\Phi_1)\rangle=-\tfrac{1}{2}$$

$$\langle\exp(i\Phi_2)\rangle=\tfrac{1}{4}(1+\tfrac{3}{4}\alpha_h-\tfrac{3}{4}\alpha_c+\tfrac{3}{4}\alpha_{hhc}-\tfrac{3}{4}\alpha_{cch}+3\alpha_{4h}-3\alpha_{4c})$$

$$\langle\exp(i\Phi_3)\rangle=-\tfrac{1}{8}(1+\tfrac{3}{4}\alpha_h-\tfrac{9}{4}\alpha_c+\tfrac{9}{4}\alpha_{hhc}-\tfrac{3}{4}\alpha_{cch}+3\alpha_{4h}+6\alpha_{2hc}-9\alpha_{4c})$$

$$\langle\exp(i\Phi_4)\rangle=-\tfrac{1}{2}(1-\tfrac{3}{4}\alpha_h-\tfrac{3}{4}\alpha_{hhc}-\tfrac{3}{4}\alpha_{cch}-3\alpha_{4h}-6\alpha_{2hc})$$

$$\langle\exp(i\Phi_5)\rangle=\tfrac{1}{8}(5-\tfrac{21}{4}\alpha_h+\tfrac{15}{4}\alpha_c-\tfrac{15}{4}\alpha_{hhc}-\tfrac{27}{4}\alpha_{cch}-12\alpha_{4h}-24\alpha_{2hc}-3\alpha_{4c}) \quad (7)$$

$$\langle\exp(i\Phi_6)\rangle=-\tfrac{1}{2}(1-\tfrac{3}{4}\alpha_h-\tfrac{9}{4}\alpha_{cch}-\tfrac{3}{2}\alpha_{4h}-\tfrac{9}{2}\alpha_{2hc}-\tfrac{3}{2}\alpha_{4c})$$

$$\langle\exp(i\Phi_7)\rangle=\tfrac{1}{8}(5-\tfrac{33}{4}\alpha_h-\tfrac{21}{4}\alpha_c+\tfrac{21}{4}\alpha_{hhc}-\tfrac{39}{4}\alpha_{cch}-9\alpha_{4h}-18\alpha_{2hc}-18\alpha_{4c}).$$

Substituting from equations (5), (6) and (7) in equation (3) and solving the resultant set of eight simultaneous equations for the C_ν's, we have

$$C_1=C_{11}^*=0{\cdot}0251\{1+1{\cdot}3274(\alpha_h-\alpha_{cch})+1{\cdot}058\alpha_{4h}-1{\cdot}616\alpha_{2hc}-0{\cdot}558\alpha_{4c}-i[0{\cdot}9330(\alpha_h+\alpha_{cch})-1{\cdot}8325\alpha_{4h}+2{\cdot}799\alpha_{2hc}-0{\cdot}9665\alpha_{4c}]\}$$

$$C_2=C_{10}^*=0{\cdot}0938\{1-0{\cdot}25(\alpha_h-\alpha_{cch})-0{\cdot}625\alpha_{4h}-0{\cdot}25\alpha_{2hc}-0{\cdot}875\alpha_{4c}+i[0{\cdot}1443(\alpha_h+\alpha_{cch})+1{\cdot}0825\alpha_{4h}+0{\cdot}433\alpha_{2hc}-1{\cdot}5155\alpha_{4c}]\}$$

Table 1. *Structure factors for hhcc crystals*

$F=0$ for $H-K+L\neq 3N$

$|F|$

$H-K$ \ L	$12M$	$12M\pm1$	$12M\pm2$	$12M\pm3$	$12M\pm4$	$12M\pm5$	$12M\pm6$
$3N$	$12f$	0	0	0	0	0	0
$3N\pm1$	0	$(3\sqrt{6}/2)(\sqrt{3}-1)f$	$3\sqrt{3}f$	0	$3f$	$(3\sqrt{6}/2)(\sqrt{3}+1)f$	0

Table 2. *Stacking faults in hhcc crystals*

Fault	Notation	Process of formation	Stacking sequence
Growth	*hhc*	Removal of 1 layer + glide	*h h c c h h c h h c c h h c* *A C B A B A C* ∣ *A C B A B A C*
	c	Insertion of 1 layer + glide	*h c c h h c c c h h c c h h* *C B A B A C B* ∣ *A B A C B C B*
	h	Twin	*c h h c c h h h c c h h c c* *C A C B A B A* ∣ *B C A C A B C*
	cch	Twin	*c c h h c c h c c h h c c h* *B A B A C B C* ∣ *A B A B C A C*
Deformation	4*h*	Glide	*c h h c c h h h h h h c c h* *C A C B A B A* ∣ *B A B A C B C*
	2*hc*	Glide	*h h c c h h c h c h c c h h* *A C B A B A C* ∣ *A B A C B C B*
	4*c*	Glide	*h c c h h c c c c c c h h c* *C B A B A C B* ∣ *A C B A B A C*

$$C_4=C_8^*=0{\cdot}0313\{1-2{\cdot}25(\alpha_h-\alpha_{cch})-1{\cdot}125\alpha_{4h}+0{\cdot}75\alpha_{2ch}-0{\cdot}375\alpha_{4c}-i[1{\cdot}8764(\alpha_h+\alpha_{cch})+1{\cdot}9486\alpha_{4h}-1{\cdot}299\alpha_{2hc}-0{\cdot}6495\alpha_{4c}]\} \quad (8)$$

$$C_5=C_7^*=0{\cdot}3499\{1+0{\cdot}1727(\alpha_h-\alpha_{cch})+0{\cdot}192\alpha_{4h}+0{\cdot}116\alpha_{2hc}+0{\cdot}308\alpha_{4c}-i[0{\cdot}067(\alpha_h+\alpha_{cch})+0{\cdot}3325\alpha_{4h}+0{\cdot}201\alpha_{2hc}-0{\cdot}5335\alpha_{4c}]\}$$

where the * denotes complex conjugation. Substituting from equations (3) and (5) in (1), we have on simplification

$$\begin{aligned}I(h_3)=\psi^2&\left[C_{1r}\sum_m Z_1^{|m|}\cos 2\pi m\left(\frac{h_3}{12}-\tfrac{1}{12}-X_1\right)-C_{1i}\sum_m Z_1^{|m|}\sin 2\pi|m|\left(\frac{h_3}{12}-\tfrac{1}{12}-X_1\right)\right]\\
+\psi^2&\left[C_{2r}\sum_m Z_2^{|m|}\cos 2\pi m\left(\frac{h_3}{12}-\tfrac{2}{12}-X_2\right)-C_{2i}\sum_m Z_2^{|m|}\sin 2\pi|m|\left(\frac{h_3}{12}-\tfrac{2}{12}-X_2\right)\right]\\
+\psi^2&\left[C_{4r}\sum_m Z_4^{|m|}\cos 2\pi m\left(\frac{h_3}{12}-\tfrac{4}{12}-X_4\right)-C_{4i}\sum_m Z_4^{|m|}\sin 2\pi|m|\left(\frac{h_3}{12}-\tfrac{4}{12}-X_4\right)\right]\\
+\psi^2&\left[C_{5r}\sum_m Z_5^{|m|}\cos 2\pi m\left(\frac{h_3}{12}-\tfrac{5}{12}-X_5\right)-C_{5i}\sum_m Z_5^{|m|}\sin 2\pi|m|\left(\frac{h_3}{12}-\tfrac{5}{12}-X_5\right)\right]\\
+\psi^2&\left[C_{5r}\sum_m Z_5^{|m|}\cos 2\pi m\left(\frac{h_3}{12}-\tfrac{7}{12}+X_5\right)+C_{5i}\sum_m Z_5^{|m|}\sin 2\pi|m|\left(\frac{h_3}{12}-\tfrac{7}{12}+X_5\right)\right]\\
+\psi^2&\left[C_{4r}\sum_m Z_4^{|m|}\cos 2\pi m\left(\frac{h_3}{12}-\tfrac{8}{12}+X_4\right)+C_{4i}\sum_m Z_4^{|m|}\sin 2\pi|m|\left(\frac{h_3}{12}-\tfrac{8}{12}+X_4\right)\right]\\
+\psi^2&\left[C_{2r}\sum_m Z_2^{|m|}\cos 2\pi m\left(\frac{h_3}{12}-\tfrac{10}{12}+X_2\right)+C_{2i}\sum_m Z_2^{|m|}\sin 2\pi|m|\left(\frac{h_3}{12}-\tfrac{10}{12}+X_2\right)\right]\\
+\psi^2&\left[C_{1r}\sum_m Z_1^{|m|}\cos 2\pi m\left(\frac{h_3}{12}-\tfrac{11}{12}+X_1\right)+C_{1i}\sum_m Z_1^{|m|}\sin 2\pi|m|\left(\frac{h_3}{12}-\tfrac{11}{12}+X_1\right)\right]\end{aligned} \quad (9)$$

where C_{vr} and C_{vi} are the real and imaginary parts of C_v and are given by

$$C_{vr}=(\tfrac{1}{2})(C_v+C_v^*);\; C_{vi}=\left(\frac{1}{2i}\right)(C_v-C_v^*)\quad v=1,2,4,5. \quad (10)$$

Performing the summations in equation (9), we have

$$\begin{aligned}I(h_3)&=\psi^2C_{1r}\frac{1-Z_1^2-2(C_{1i}/C_{1r})Z_1\sin 2\pi\left(\frac{h_3}{12}-\frac{1}{12}-X_1\right)}{1+Z_1^2-2Z_1\cos 2\pi\left(\frac{h_3}{12}-\frac{1}{12}-X_1\right)}\\
&+\psi^2C_{2r}\frac{1-Z_2^2-2(C_{2i}/C_{2r})Z_2\sin 2\pi\left(\frac{h_3}{12}-\frac{2}{12}-X_2\right)}{1+Z_2^2-2Z_2\cos 2\pi\left(\frac{h_3}{12}-\frac{2}{12}-X_2\right)}\\
&+\psi^2C_{4r}\frac{1-Z_4^2-2(C_{4i}/C_{4r})Z_4\sin 2\pi\left(\frac{h_3}{12}-\frac{4}{12}-X_4\right)}{1+Z_4^2-2Z_4\cos 2\pi\left(\frac{h_3}{12}-\frac{4}{12}-X_4\right)}\\
&+\psi^2C_{5r}\frac{1-Z_5^2-2(C_{5i}/C_{5r})Z_5\sin 2\pi\left(\frac{h_3}{12}-\frac{5}{12}-X_5\right)}{1+Z_5^2-2Z_5\cos 2\pi\left(\frac{h_3}{12}-\frac{5}{12}-X_5\right)}\\
&+\psi^2C_{5r}\frac{1-Z_5^2+2(C_{5i}/C_{5r})Z_5\sin 2\pi\left(\frac{h_3}{12}-\frac{7}{12}+X_5\right)}{1+Z_5^2-2Z_5\cos 2\pi\left(\frac{h_3}{12}-\frac{7}{12}+X_5\right)}\\
&+\psi^2C_{4r}\frac{1-Z_4^2+2(C_{4i}/C_{4r})Z_4\sin 2\pi\left(\frac{h_3}{12}-\frac{8}{12}+X_4\right)}{1+Z_4^2-2Z_4\cos 2\pi\left(\frac{h_3}{12}-\frac{8}{12}+X_4\right)}\\
&+\psi^2C_{2r}\frac{1-Z_2^2+2(C_{2i}/C_{2r})Z_2\sin 2\pi\left(\frac{h_3}{12}-\frac{10}{12}+X_2\right)}{1+Z_2^2-2Z_2\cos 2\pi\left(\frac{h_3}{12}-\frac{10}{12}+X_2\right)}\\
&+\psi^2C_{1r}\frac{1-Z_1^2+2(C_{1i}/C_{1r})Z_1\sin 2\pi\left(\frac{h_3}{12}-\frac{11}{12}+X_1\right)}{1+Z_1^2-2Z_1\cos 2\pi\left(\frac{h_3}{12}-\frac{11}{12}+X_1\right)}.\end{aligned} \quad (11)$$

Description of diffraction effects

Reflexions with $H-K=3N$, $L=12M$, M and N integers, remain sharp. For reflexions with $H-K\neq 3N$, the first to eighth terms on the right-hand side of equation (11) give rise to broadened peaks corresponding to $L=12M+1$, $12M+2$, $12M+4$, $12M+5$, $12M+7$, $12M+8$, $12M+10$, $12M+11$ respectively. In general, all reflexions exhibit changes in integrated intensity, profile peak shift, profile broadening and profile asymmetry. These effects can be utilized for estimating fault probabilities. Quantitative expressions for these profile characteristics are given below.

Profile integrated intensity

The integrated intensities T_1, T_2, T_4 and T_5 in reciprocal space for reflexions with $L=12M\pm1$, $12M\pm2$, $12M\pm4$ and $12M\pm5$ respectively can be obtained by integrating separately the corresponding terms on the right-hand side of equation (11) with respect to h_3. The fractional changes in the ratios R_{21}, R_{41} and R_{51} of the integrated intensities (T_2, T_1), (T_4, T_1) and (T_5, T_1) respectively are given by

$$\Delta R_{21}/R_{21} = -1\cdot5774(\alpha_h-\alpha_{cch})-1\cdot683\alpha_{4h} + 1\cdot366\alpha_{2hc}-0\cdot317\alpha_{4c} \quad (12)$$

$$\Delta R_{41}/R_{41} = -3\cdot5774(\alpha_h-\alpha_{cch})-2\cdot183\alpha_{4h} + 2\cdot366\alpha_{2hc}+0\cdot183\alpha_{4c} \quad (13)$$

$$\Delta R_{51}/R_{51} = -1\cdot1547(\alpha_h-\alpha_{cch})-0\cdot866\alpha_{4h} + 1\cdot732\alpha_{2hc}+0\cdot866\alpha_{4c}\,. \quad (14)$$

By experimental measurement of the quantities $\Delta R_{21}/R_{21}$, $\Delta R_{41}/R_{41}$ and $\Delta R_{51}/R_{51}$, one obtains three different combinations of the fault probabilities. We designate such linear combinations by the term compound fault parameter.

Profile peak shift

Each term on the right-hand side of equation (11) gives rise to a peak when the argument of the cosine term in the denominator is a multiple of 2π. Thus the changes in the profile peak positions due to faulting can be found and after conversion to $2\theta^\circ$ coordinates are given by

$$\Delta(2\theta_m)_1^\circ = \mp \frac{270}{\pi^2}\cdot\frac{|L|d^2}{c^2}\cdot\tan\theta\{(\alpha_c-\alpha_{hhc}) + \sqrt{3}(\alpha_{4h}+2\alpha_{2hc}-\alpha_{4c})\} \quad \text{for } L=12M\pm1 \quad (15)$$

$$\Delta(2\theta_m)_2^\circ = \pm \frac{270}{\pi^2}\cdot\frac{|L|d^2}{c^2}\cdot\tan\theta\{\sqrt{3}(\alpha_c-\alpha_{hhc}) + \sqrt{3}(\alpha_{4h}+2\alpha_{2hc}-\alpha_{4c})\} \quad \text{for } L=12M\pm2 \quad (16)$$

$$\Delta(2\theta_m)_4^\circ = \pm \frac{270}{\pi^2}\cdot\frac{|L|d^2}{c^2}\cdot\tan\theta\{\sqrt{3}(\alpha_c-\alpha_{hhc}) - \sqrt{3}(\alpha_{4h}+2\alpha_{2hc}-\alpha_{4c})\} \quad \text{for } L=12M\pm4 \quad (17)$$

$$\Delta(2\theta_m)_5^\circ = \mp \frac{270}{2}\cdot\frac{|L|d^2}{c^2}\cdot\tan\theta\{(\alpha_c-\alpha_{hhc}) - \sqrt{3}(\alpha_{4h}+2\alpha_{2hc}-\alpha_{4c})\} \quad \text{for } L=12M\pm5\,. \quad (18)$$

Profile peak shift measurements thus lead to estimates of four more compound fault parameters. However, only two of these are independent.

Profile integral breadth

The integral breadth is defined as the ratio of the profile integrated intensity and the profile maximum. Considering each of the terms in equation (11) separately and converting to $2\theta^\circ$ coordinates we have

$$(\beta_f)_1^\circ = \frac{270}{\pi}\cdot\frac{|L|d^2}{c^2}\cdot\tan\theta\{2(\alpha_h+\alpha_{cch})+(2+\sqrt{3}) \times(\alpha_c+\alpha_{hhc})+3(\alpha_{4h}+2\alpha_{2hc}+\alpha_{4c})\} \quad \text{for } L=12M\pm1 \quad (19)$$

$$(\beta_f)_2^\circ = \frac{270}{\pi}\cdot\frac{|L|d^2}{c^2}\cdot\tan\theta\{2(\alpha_h+\alpha_{cch})+(\alpha_c+\alpha_{hhc}) +3(\alpha_{4h}+2\alpha_{2hc}+\alpha_{4c})\} \quad \text{for } L=12M\pm2 \quad (20)$$

$$(\beta_f)_4^\circ = \frac{270}{\pi}\cdot\frac{|L|d^2}{c^2}\cdot\tan\theta\{2(\alpha_h+\alpha_{cch})+3(\alpha_c+\alpha_{hhc}) +3(\alpha_{4h}+2\alpha_{2hc}+\alpha_{4c})\} \quad \text{for } L=12M\pm4 \quad (21)$$

$$(\beta_f)_5^\circ = \frac{270}{\pi}\cdot\frac{|L|d^2}{c^2}\cdot\tan\theta\{2(\alpha_h+\alpha_{cch})+(2-\sqrt{3}) \times(\alpha_c+\alpha_{hhc})+3(\alpha_{4h}+2\alpha_{2hc}+\alpha_{4c})\} \quad \text{for } L=12M\pm5\,. \quad (22)$$

Four additional compound fault parameters can, therefore, be obtained from measurements of $(\beta_f)_1^\circ$, $(\beta_f)_2^\circ$, $(\beta_f)_4^\circ$ and $(\beta_f)_5^\circ$. Again, however, only two of these are independent.

Profile asymmetry

A simple measure of profile asymmetry is the shift of the centroid of a profile from its peak position. Following Cohen & Wagner (1962), we have from equation (9)

$$\Delta(2\theta_{c-m})_1^\circ = \pm\frac{360\ln 2}{\pi^2}\cdot\tan\theta\{0\cdot933(\alpha_h+\alpha_{cch}) -1\cdot8325\alpha_{4h}+2\cdot799\alpha_{2ch}-0\cdot9665\alpha_{4c}\} \quad \text{for } L=12M\pm1 \quad (23)$$

$$\Delta(2\theta_{c-m})_2^\circ = \pm\frac{360\ln 2}{\pi^2}\cdot\tan\theta\{-0\cdot1443(\alpha_h+\alpha_{cch}) -1\cdot0825\alpha_{4h}-0\cdot433\alpha_{2ch}+1\cdot5155\alpha_{4c}\} \quad \text{for } L=12M\pm2 \quad (24)$$

$$\Delta(2\theta_{c-m})_4^\circ = \pm\frac{360\ln 2}{\pi^2}\cdot\tan\theta\{1\cdot8764(\alpha_h+\alpha_{cch}) +1\cdot9486\alpha_{4h}-1\cdot299\alpha_{2ch}-0\cdot6495\alpha_{4c}\} \quad \text{for } L=12M\pm4 \quad (25)$$

$$\Delta(2\theta_{c-m})_5^\circ = \pm\frac{360\ln 2}{\pi^2}\cdot\tan\theta\{0\cdot067(\alpha_h+\alpha_{cch}) +0\cdot3325\alpha_{4h}+0\cdot201\alpha_{2hc}-0\cdot5335\alpha_{4c}\} \quad \text{for } L=12M\pm5\,. \quad (26)$$

Thus, measurement of asymmetry leads to estimates of four more compound fault parameters.

Discussion

Independent estimates of a total of eleven compound fault parameters can be obtained from measurements of the profile characteristics mentioned above. Since there are only seven fault probabilities, we have an overdetermined set of equations and, in principle, all seven fault probabilities can be found. In practice, all the data required may not be available with sufficient accuracy and further the profile broadening may include effects due to small domains and lattice strains within the specimen. Analysis of the broadening data is more complicated for this structure (as also the *hcc* structure) since the first two fault-unaffected reflexions, namely 00012 and $11\bar{2}0$ are superimposed on fault-affected reflexions, namely $10\bar{1}4$ and $10\bar{1}16$. A method similar in principle to that outlined previously for the *hcc* structure may, however, be utilized for an approximate analysis (Lele, 1974*a*).

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APPENDIX

Characteristic equation for deformation faults

We consider four types of layers to be present in the perfect *hhcc* structure according as they continue the stacking in an *hh*, *ch*, *cc* or *hc* way. We further note that 4*h* and 4*c* faults can occur only after *hh* and *cc* layers respectively while 2*hc* faults can occur after *hc* and *ch* layers only (Table 2). The transition probabilities as also the phase differences from the $(m-1)$ to the m layer for the above four types of layer are shown in Table 3. Let Φ_m^y represent the phase difference for an m layer of the type y from the origin layer, where y represents one of *hh*, *ch*, *cc* and *hc*. Then from Table 3 we have

$$\langle\exp(i\Phi_m^{hh})\rangle=\{(1-\alpha_{2hc})\omega^*+\alpha_{2hc}\omega\}\langle\exp(i\Phi_{m-1}^{ch})\rangle \qquad (A1)$$

$$\langle\exp(i\Phi_m^{ch})\rangle=\{(1-\alpha_{4c})\omega+\alpha_{4c}\omega^*\}\langle\exp(i\Phi_{m-1}^{cc})\rangle \qquad (A2)$$

$$\langle\exp(i\Phi_m^{cc})\rangle=\{(1-\alpha_{2hc})\omega^*+\alpha_{2hc}\omega\}\langle\exp(i\Phi_{m-1}^{hc})\rangle \qquad (A3)$$

$$\langle\exp(i\Phi_m^{hc})\rangle=\{(1-\alpha_{4h})\omega^*+\alpha_{4h}\omega\}\langle\exp(i\Phi_{m-1}^{4h})\rangle \qquad (A4)$$

where

$$\omega=\exp(2\pi i/3)(H-K)=\exp(i\varphi_0)\,. \qquad (A5)$$

Replacing m by $(m-1)$, $(m-2)$ and $(m-3)$ in equations $(A2)$, $(A3)$ and $(A4)$ respectively and eliminating $\langle\exp(i\Phi_{m-1}^{ch})\rangle$, $\langle\exp(i\Phi_{m-2}^{cc})\rangle$ and $\langle\exp(i\Phi_{m-3}^{hc})\rangle$ among the resulting equations and equation $(A1)$, we obtain

$$\langle\exp(i\Phi_m^{hh})\rangle=\{(1-\alpha_{2hc})\omega^*+\alpha_{2hc}\omega\}^2 \times\{(1-\alpha_{4c})\omega+\alpha_{4c}\omega^*\} \times\{(1-\alpha_{4h})\omega^*+\alpha_{4h}\omega\}\langle\exp(i\Phi_{m-4}^{hh})\rangle\,. \qquad (A6)$$

Let the solution of this recurrence equation be of the form

$$\langle\exp(i\Phi_m^{hh})\rangle=C\varrho^m. \qquad (A7)$$

Substituting from equation $(A7)$ in $(A6)$, we get

$$\varrho^4-\{(1-\alpha_{2hc})\omega^*+\alpha_{2hc}\omega\}^2\{(1-\alpha_{4c})\omega+\alpha_{4c}\omega^*\} \times\{(1-\alpha_{4h})\omega^*+\alpha_{4h}\omega\}=0\,. \qquad (A8)$$

It can be shown that, for crystals in the twin orientation, the complex conjugate of the above equation holds. Thus

$$\varrho^4-\{(1-\alpha_{2hc})\omega+\alpha_{2hc}\omega^*\}^2\{(1-\alpha_{4c})\omega^*+\alpha_{4c}\omega\} \times\{(1-\alpha_{4h})\omega+\alpha_{4h}\omega^*\}=0\,. \qquad (A9)$$

The same relations can be shown to hold for the other types of layers. For a crystal simultaneously containing *h* and/or *hcc* faults (which arise from twinning operations, Table 2), some regions of the crystal are in the normal orientation and others in the twin orientation. An equation applicable in this situation is obtained by multiplying equations $(A8)$ and $(A9)$ giving on simplification

$$\varrho^8+(1-3\alpha_{4h}-6\alpha_{2hc})\varrho^4 +(1-3\alpha_{4h}-6\alpha_{2hc}-3\alpha_{4c})=0 \quad \text{for } \alpha\text{'s}\ll 1 \qquad (A10)$$

where terms with squares and higher powers of the fault probabilities as well as their cross products have been omitted.

Table 3. *Probability trees giving transition probabilities and phase differences from one layer to the next*

$(m-1)$ layer	Probability	m layer	Phase difference
ch A	$1-\alpha_{2hc}$	*hh* C	$-\varphi_0$
	α_{2hc}	*hh* B	$+\varphi_0$
cc A	$1-\alpha_{4c}$	*ch* B	$+\varphi_0$
	α_{4c}	*ch* C	$-\varphi_0$
hc A	$1-\alpha_{2hc}$	*cc* C	$-\varphi_0$
	α_{2hc}	*cc* B	$+\varphi_0$
hh A	$1-\alpha_{4h}$	*hc* C	$-\varphi_0$
	α_{4h}	*hc* B	$+\varphi_0$

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Ambiguities in the X-ray Analysis of Crystal Structures*

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A mathematical construction is given for arbitrarily many distinct crystal structures all of which would give the same diffraction pattern. A. L. Patterson's concept of *homometric sets* is analyzed, and examples are given in one, two and three dimensions.

Let $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ be linearly independent vectors in three-dimensional space. Let A be the three-by-three matrix whose columns are the $\mathbf{a}_j$. The vectors $\mathbf{a}_j$ determine a *lattice* of points

$$\mathsf{A}\mathbf{n} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \tag{1}$$

where the n_j are integers. The *basic cell* of the lattice is the set of points

$$\mathbf{x} = \xi_1\mathbf{a}_1 + \xi_2\mathbf{a}_2 + \xi_3\mathbf{a}_3 \text{ with } 0 \le \xi_j < 1 \; . \tag{2}$$

The *reciprocal lattice* has the matrix

$$\mathsf{B} = (\mathsf{A}^T)^{-1} = (\mathsf{A}^{-1})^T \; . \tag{3}$$

Its columns $\mathbf{b}_j$ satisfy

$$\begin{aligned} \mathbf{a}_k \,.\, \mathbf{b}_j = \delta_{kj} &= 0 \text{ if } k \ne j \\ &= 1 \text{ if } k = j \; . \end{aligned} \tag{4}$$

The reciprocal lattice consists of the points $\mathsf{B}\mathbf{h}$, where the h_j are integers (called Miller indices).

Let the atoms in a crystal be located at $\mathbf{r}_1, \ldots, \mathbf{r}_N$ in the basic cell (2) and at all *congruent* points $\mathbf{r}_j + \mathsf{A}\mathbf{n}$. By X-ray analysis, one tries to find the positions $\mathbf{r}_j$.

The F factor is defined to be

$$F(\mathbf{h}) = \sum_{s=1}^{N} f_s \exp 2\pi i\, \mathbf{h} \,.\, \mathbf{r}_s \; . \tag{5}$$

For $\mathbf{h}$ in the reciprocal lattice, observations are made of

$$|F(\mathbf{h})|^2 = \sum_{s=1}^{N} \sum_{t=1}^{N} f_s f_t \exp 2\pi i \mathbf{h} \,.\, (\mathbf{r}_t - \mathbf{r}_s) \; . \tag{6}$$

The f_s are positive numbers.

If the F factors were observed, the $\mathbf{r}_s$ would be determined uniquely. Ambiguity results from observing $|F^2|$ instead of F.

In the following definitions, let X,Y,... represent finite non-empty point sets in the real Euclidian space of n dimensions. A set X is allowed to have repeated elements, but no ordering or indexing is prescribed. For instance, if $\mathsf{X} = \{1,1,2\}$ in one dimension, then

$$\mathsf{X} = \{1,2,1\} \quad \text{but} \quad \mathsf{X} \ne \{1,2\} \; .$$

Given X and Y, we define the sets

$$\begin{aligned} \mathsf{X}+\mathsf{Y} &= \{\mathbf{x}+\mathbf{y}\} \; (\mathbf{x} \text{ in } \mathsf{X}, \mathbf{y} \text{ in } \mathsf{Y}) \\ \lambda\mathsf{X} &= \{\lambda\mathbf{x}\} \; (\mathbf{x} \text{ in } \mathsf{X}) \\ -\mathsf{X} &= \{-\mathbf{x}\} \; (\mathbf{x} \text{ in } \mathsf{X}) \\ \mathsf{X}+\mathbf{c} &= \{\mathbf{x}+\mathbf{c}\} \; (\mathbf{x} \text{ in } \mathsf{X}) \\ \mathsf{X}-\mathsf{Y} &= \mathsf{X}+(-\mathsf{Y}) = \{\mathbf{x}-\mathbf{y}\} \\ \mathsf{D}(\mathsf{X}) &= \mathsf{X}-\mathsf{X} \; . \end{aligned} \tag{7}$$

Thus, if X has m members, D(X) has m^2 members, including at least m points $\mathbf{0}$.

Suppose

$$\mathsf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\} \text{ and } \mathsf{Y} = \{\mathbf{y}_1, \ldots, \mathbf{y}_m\} \; . \tag{8}$$

We say

$$\mathsf{X} = \mathsf{Y} \text{ if}$$
$$\mathbf{x}_1 = \mathbf{y}_{j1}, \ldots, \mathbf{x}_m = \mathbf{y}_{jm}$$

where $j_1, \ldots, j_m$ is some permutation of $1, \ldots, m$.

Let $\mathbf{x}$ and $\mathbf{y}$ be points in real n-dimensional space.

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